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Creating a Simple Single Computational Approach to Modeling Rarefied and Continuum Flow About Aerospace Vehicles

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Summary

We proposed to create a single computational code incorporating methods that can model both rarefied and continuum flow to enable the efficient simulation of flow about space craft and high altitude hypersonic aerospace vehicles. The code was to use a single grid structure that permits a smooth transition between the continuum and rarefied portions of the flow. Developing an appropriate computational boundary between the two regions represented a major challenge. The primary approach chosen involves coupling a four-speed Lattice Boltzmann model for the continuum flow with the DSMC method in the rarefied regime. We also explored the possibility of using a standard finite difference Navier Stokes solver for the continuum flow. With the resulting code we will ultimately investigate three-dimensional plume impingement effects, a subject of critical importance to NASA and related to the work of Drs. Forrest Lumpkin, Steve Fitzgerald and Jay Le Beau at Johnson Space Center.

Below is a brief background on the project and a summary of the results as of the end of the grant.

Calculating Transitional Regime Flows

Plume flows near spacecraft contain both continuum and rarefied regions. While there are many different approaches to modeling each region separately, there is presently no single approach that can simultaneously model both regions efficiently and accurately. Having a single computational code that can handle both regions is important because the flows may be unsteady, there may be multiple interacting regions of rarefied/continuum flow, there can be subsonic overlap regions, or the flow computation must reach a steady state through an interacting relaxation process during which the different regions exchange information. In these cases the use of two separate computer codes is not only awkward and error-prone but also inefficient due to the need to swap and convert data between the codes after every time step. This is particularly so because the codes may not represent the fluid in the same way.

In a fully continuum flow the integration of the Navier Stokes (NS) equations is a well established practice [1]. For lower density flows, however, the NS equations no longer apply. The Burnett equations may be used to extend the applicability of the NS equations further into the rarefied regime [2]. However, the most practical approach for modeling rarefied flow is the Direct Simulation Monte Carlo (DSMC) method of Bird [3] in which Lagrangian molecules are collided and moved to model the flowing gas. The computational cost in DSMC is proportional to the number of molecules simulated. To model transitional flow, for example continuum-to-rarefied plume flow expansions, the DSMC has been used all the way into the nozzle throat. In fact, this is one approach studied at JSC by Jay Le Beau in the Aeroscience Branch of the Navigation, Control and Aeronautics Division. However, except for very small plumes [4], it has been impractical to use full resolution for the DSMC simulations inside the nozzle. Thus, for purposes of computing the far field low density flow, the continuum flow was only crudely modeled by DSMC.

Merging Continuum and DSMC Codes

We are developing a hybrid computational code which can handle unsteady transitional flows containing both fully rarefied and fully continuum regions (i.e., the flow field in and around a thruster during startup). To do this we are merging the DSMC and a continuum procedure into a single routine. This work has centered around developing the interface between the two different representations of a flow: macroscopic parameters ($\vec{U}$, ρ, T etc.) in the continuum flow and the microscopic particle velocity distribution functions in the rarefied flow. For unsteady and subsonic flows it is essential that the flow information be free to propagate in either direction, i.e., rarefied to continuum or continuum to rarefied. It is also desirable that both types of code be compatible with future vector and parallel supercomputer architectures.

We have been working on the project with PhD students who have passed the doctoral qualifying exam and have had JSC funding since June, 1995. First, we explored a range of code combinations since it was not obvious which types of codes should be merged. One combination appeared well suited to the problems of interest: the Lattice Boltzmann Equation (LBE) discrete-velocity approach [5,6] for use in the continuum region and the DSMC approach in the transitional and rarefied regions. The advantages of using the discrete-velocity gas model are that then the representation of the flow in terms of velocity distribution func-

tions and particles is similar in both flow regimes. In addition, it may be possible to compute flows more quickly using less memory than with an ordinary finite difference representation of the continuum flow.

Recently, the continuum Euler equations have been solved using a discrete-velocity distribution function model based on a local thermodynamic equilibrium assumption. This LBE method is termed the Adaptive Discrete Velocity (ADV) method of Nadiga [7]. The approach uses a flux-splitting/TVD scheme based on Nadiga and Pullin's Flux-splitting Equilibrium Method [8]. The ADV approach obviates the need for the expensive computation of the Lattice Boltzmann collision integral by assuming an equilibrium distribution function based on macroscopic properties at each cell center. However, the method is also unique in that it retains a non-equilibrium distribution function at cell boundaries because of the superposition of fluxes arising from neighboring cells with possibly different properties. The ADV approach appears to allow an efficient coupling between continuum and rarefied regions by combining a quasi-particle approach with a true particle simulation.

Hence, we have chosen to merge the DSMC and ADV/LBE approaches because: a) DSMC is the most common, flexible, and well tested solver for the rarefied flow regime, b) the ADV approach provides a suitable representation of discrete distribution functions to interface with the DSMC, c) the work greatly benefits from on-going collaboration with Dr. Nadiga at the Los Alamos National Laboratory, d) the ADV approach is a reasonably efficient and stable approach to solving the continuum flow, and e) both methods maintain similar references to distribution functions and proceed through related move-collide-move and flux-equilibrate-flux sequences. On the other hand, finite difference/volume NS solvers are now industrial standard approaches having well documented features and limitations. Thus, we are developing an interface that is not entirely specific to the ADV and DSMC codes and should be more broadly applicable to merge other NS solvers with DSMC.

Results

As part of this grant we have developed suitable versions of the DSMC and ADV codes and have created a reasonably satisfactory but simple interface. The interface consists of a layered set of reservoir cells, buffer cells and ghost cells (Fig. 1). The particles which enter the DSMC region are generated from the equilibrium ADV properties in the two ADV cells bounding the DSMC region. The boundary cells in the ADV domain (ADV buffer cells) similarly utilize the macroscopic properties in the two bounding DSMC cells to obtain the DSMC-to-ADV fluxes. Because the ADV method is second order in time and uses half-step properties, a form of half-step DSMC is done in the boundary cells. To obtain smooth time-accurate inputs to the ADV region, there is a portion of the DSMC region along the boundary in which 'ghost-cells' are used. Within the ghost-cells essentially an $n-$parallel DSMC computation occurs in which the n ghost levels compute statistically somewhat independent problems.[1] Particles entering the ghost region are cloned n times while those departing for the ordinary DSMC side are destroyed with probability $n/(n+1)$. Those which leave for the ADV side are lost altogether. Hence, we may compute with 40

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[1]The problems are not truly independent because each ghost level has cloned particles as inputs.

particles per cell in most of a DSMC region while, with 10 levels of ghost-cells ($n = 10$), the ADV buffer cells see a random noise level closer to that found with 400 particles per cell. Presently we use a rectilinear Cartesian grid in both regions although the cell sizes may differ across the boundary. A set of grid maps are used to delineate the different regions and cell types.

Consider some example results illustrating the use of the hybrid code. See the figure caption page for details of each simulation. Figure 2 shows the unsteady passage of a normal shock wave through the interface. The passage occurs smoothly with no apparent reflected waves and the proper shock jump conditions are maintained. Notice the change is shock slope between the two methods: whereas DSMC fully resolves the wave, the Euler solution of the ADV method produces a wave whose thickness (roughly 3 cells) is controlled by second order numerical viscosity. Passage of rarefactions is equally uneventful. Figure 3 illustrates the passage of a shear "wave" through the interface. The problem solved is the strongly compressible Rayleigh problem: a diffusely reflective flat plate was abruptly moved in its own plane. This generated weak shocks and rarefactions which quickly left the scene. Much later, as seen in the figure, the diffusively growing shear layer gradually penetrates the interface and experiences a slope discontinuity due to the inconsistent nature of the problem (nearly an Euler/inviscid solution on the ADV side). This example illustrates that the interface should remain within the nearly inviscid flow to avoid such errors. Figure 4 illustrates the use of DSMC to capture a rarefied flow effect within an otherwise continuum flow. A Mach 3 shock wave is captured by DSMC while ADV computes the upstream and downstream regions. The quieting effect of the ghost cells is evident. Figure 5 presents preliminary results for a simple plume impingement problem. A small plume, generated by a 10 to 1 pressure difference across a 2D narrow slot, strikes a flat plate 6 slot heights downstream. This problem demonstrates several features of our approach: (1) solid surfaces on which boundary layers may be important are within the DSMC domains, (2) multiple detached domains can be used, (3) interfaces can be placed in sub- or supersonic flow, (4) oblique wave passage through the interfaces is uneventful, (5) continuum code can be used to handle subsonic domain boundaries, and (6) reasonable solutions can be obtained with minimal ensemble averaging. A video tape containing the unsteady development of this flow has been sent to Dr. Lumpkin.

Finally, we point out that a detailed description of the work was presented at the 35th Aerospace Sciences meeting in Reno, NV in January, 1997 as paper 97-1006. This paper is being prepared for submission to a journal and has been sent to Mr. Cones by surface mail.

References

[1] D. Anderson, J, Tannehill and R. Pletcher, *Computational Fluid Mechanics and Heat Transfer*, Hemisphere Pub. Co., 1984.

[2] F. E. Lumpkin and D. R. Chapman, "Accuracy of the Burnett Equations for Hypersonic Real Gas Effects," AIAA meeting, Reno, Nevada, 1991. AIAA paper 91-0771.

[3] G. A. Bird, *Molecular Gasdynamics.*, Clarendon Press, Oxford, 1976.

[4] I. Boyd, Y. Jafry, and J. V. Beukel, "Investigation of Nozzle and Plume Expansions of a Small Helium Thruster," paper IA4 at the 18th Int. Symp. on Rarefied Gas Dynamics, Univ. B. C., Vancouver, B. C., July 1992. To appear in the proceedings.

[5] D. Martinez, W. Mattaeus, S. Chen, and D. Montgomery, "Comparison of Spectral Method and Lattice Boltzmann Simulations of Two-Dimensional Hydrodynamics," sub. to *Phys. Fluids A*, Feb. 1993.

[6] G. R. McNamera, and G. Zanetti, "Use of the Boltzmann Equation to Simulate Lattice Gas Automata," *Phys. Rev. Let.*, **61**, 2332-2335, 1988.

[7] B. T. Nadiga, "An adaptive discrete velocity model for the shallow water wave equations," Los Alamos report LA-UR-94-2027.

[8] B. T. Nadiga and D. I. Pullin, "A method for near-equilibrium discrete-velocity gas flows," *J. Comp. Physics*, **112**, 162 (1994).

[9] W. Feiereisen and J. McDonald, "Three Dimensional Discrete Particle Simulation of an AOTV," *Presented at the Thermophysics Conference*, Buffalo, NY, June 12-14 1989. AIAA paper: 89-1711 (1989).

[10] J. McDonald and D. Baganoff, "Vectorization of a Particle Simulation Method for Hypersonic Rarefied Flow," *Presented at the Thermophysics Conference*, San Antonio, TX, June 1988, AIAA paper: 88-2735 (1988).

[11] M. Woronowicz and J. McDonald, "Application of a Vectorized Particle Simulation in High-Speed Near-Continuum Flow," *Presented at the Thermophysics Conference*, Buffalo, NY, June 12-14 1989. AIAA paper: 89-1665 (1989).

[12] K. Kawasaki, "Monte Carlo Calculation of the Flow of Granular Materials", Engineering thesis, Calif. Inst. of Tech., 1985.

[13] D. Goldstein, "Near Continuum Applications of a Discrete-Velocity Gas Model." *Rarefied Gas Dynamics* ed. A. E. Beylich, *In Proceedings of 17th International Symposium on Rarefied Gas Dynamics*, Aachen, FRG, 1990. VCH Verlagsgesellschaft, FRG (1990)

[14] D. Goldstein and B. Sturtevant, "Discrete Velocity Gasdynamics Simulations in a Parallel Processing Environment." *Presented at the Thermophysics Conference*, Buffalo, NY, June 12-14 1989. AIAA paper: 89-1668 (1989).

[15] D. Goldstein and B. Nadiga, "Compressible Channel Flow Using Two Discrete-Velocity Gas Models," paper AB4 at the 18th Int. Symp. on Rarefied Gas Dynamics, Univ. B. C., Vancouver, B. C., July 1992. To appear in the proceedings.

[16] D. Goldstein, "Investigations of a Discrete-Velocity Gas," California Institute of Technology PhD thesis, 1990.

[17] A. Carlson and R. Wilmoth, "Monte Carlo Simulation of a Near-Continuum Shock-Shock Interaction Problem," *Presented at the Thermophysics Conference*, Nashville, TN, June 1992. AIAA paper: 98-2862 (1992).

[18] J. D. Sterling and S. Chen, "Stability Analysis of Lattice Boltzmann Methods," Los Alamos report LA-UR:93-2130.

[19] J. V. Austin and D. B. Goldstein, Direct numerical simulation of the atmosphere of Io," paper presented at (& in proc. of) NATO Adv. Studies Inst. *Molecular Phys. & Hypersonic Flows*, Maratea, Italy, May, 1995.

[20] Z. Tan and P. Varghese, "The $\Delta - \epsilon$ method for the Boltzmann equation," *J. Comp. Physics*, **110**, 327 (1994).

Figure Captions

Figure 1. Interface Configuration.

The follwing information applies to all four hybrid ADV/DSMC simulations in the following figures. "Test conditions" indicate atmospheric density at 80 km altitude (9.2e-6 kg/m^3) and a temperature of 500 K. The grids employ equi-sized ADV and DSMC cells measuring 0.8 rest mean free paths per side for figures 2,4,5 and 0.5 rest mean free paths per side for figures 3. DSMC hard sphere particles have the mass of nitrogen molecules. All solutions are advanced with time steps measuring 1×10^{-6} seconds and all were done on a DEC Alpha 3000/700 workstation.

Figure 2. Moving Normal Shock Wave. Figure 2 shows 11 realizations from a hybrid ADV/DSMC simulation of a normal shock wave passing through the interface.

The whole domain consists of 80 DSMC cells adjacent to a specular wall on the right hand side of the domain, and 52 ADV cells to the left of the interface. We further subdivide the DSMC region into 20 ghost cells, $n = 5$, near the ADV/DSMC interface. Each cell has 200 simulated molecules upstream of the shock. Thirty minutes were required to advance the computation through the 1000 time steps shown.

Flow initially moves uniformly toward the solid wall at 400 m/s (Mach 1.6). We initialize the constant upstream inflow to test conditions. Periodic boundary conditions are applied in the y direction.

The shock thickness spans about 12 rest mean free paths in the DSMC region, whereas in the ADV region it is thinned considerably and has a finite thickness only due to the effect of numerical viscosity. The solution yields the correct Rankine- Hugoniot density ratio. In the ghost cells the five-fold increase in ghost particles produces a clear reduction in noise.

Figure 3. Compressible Rayleigh Problem. Figure 3 shows tangential velocity profiles beside a flat plate suddenly moved in its own plane.

This flow demonstrates the nature of shear waves passing through the ADV/DSMC interface. We compare two hybrid DSMC/ADV solutions with differing DSMC domains. The whole domain consists of 400 cells. One computation (dashed curve) uses 280 DSMC cells adjacent to the specular wall whereas the second computation uses only 80 DSMC cells. Both DSMC domains use 20 ghost cells, $n = 5$, near the ADV/DSMC interface. Each DSMC cell is initialized with 200 simulated molecules. The solution is advanced through 10000 iterations, three of which are plotted after 200, 6000 and 10000 steps. Thirty minutes of computation time were needed.

Periodic boundary conditions are applied in the vertical direction while in the horizontal direction an absorbing boundary condition is imposed at the left side of the ADV domain. The plate at the right side of the DSMC domain is suddenly moved in its own plane to 2000 m/s (Mach 4) at $t = 0$.

There exists a small velocity slip adjacent to the wall. The full DSMC simulation captures the type of decay to the farfield value (zero u velocity) similar to that in the incompressible Rayleigh problem. The choice of collision cross section determines the viscosity in the DSMC method whereas only numerical viscosity affects the ADV result. The discontinuity in viscosity at the interface leads to thinning of the viscous region and a corresponding increase of the velocity gradient in the ADV.

Figure 4. Steady Shock. Figure 4 shows 47 overlaid realizations from a simulation of a stationary, normal shock wave.

We initialize each of the 62 DSMC cells with 800 simulated molecules upstream and 2400 downstream of the shock. Two DSMC border ghost zones (12 cells wide, $n = 5$ levels per cell) provide smooth data to the surrounding ADV regions. The solution is advanced through 5000 time steps and took 30 minutes.

Rankine-Hugoniot equations determine the boundary conditions in the x direction while periodic boundary conditions are applied in the y-direction. We initialize the Mach 3 upstream inflow conditions to test conditions. The simulation yields the correct perfect gas density ratio (3.0), as expected and the correct shock shape. The shock half-slope thickness spans approximately 4 rest mean free paths.

The effect of ghost cells is clearly visible at either end of the DSMC domain. The five-fold increase in ghost particles produces the expected 56% noise reduction. The exponential behavior of the noise in the ghost zone near the left interface arises due to cloning of incoming equilibrium particles through all n levels. Collisions in the cells downstream of the interface destroy the cloned identity, leading to noise reduction in the averaging procedure. Since the upstream flow is highly supersonic, noise propagation occurs only in the subsonic downstream ADV region.

Figure 5. Supersonic Jet Flow Impinging on a Vertical Flat Plate. Figure 5 shows pressure contours (Fig. 5a) from a 2D calculation of supersonic jet flow impinging on a vertical flat plate.

Two separate DSMC patches, embedded in the ADV domain, contain the slit vertical walls and the target plate, respectively (Fig. 5b). The whole domain (152*84 cells) consists of 2706 DSMC cells and 10062 ADV cells. We model the slit with two vertical specularly reflecting walls on either side of a centered opening 9.6 rest mean free paths (12 cells) high. The specularly reflecting target plate measures 4.8 rest mean free paths (6 cells) high and is positioned 60 rest mean free paths (75 cells) to the left of the slit.

To create a starting pressure ratio of 10:1, we initialize the DMSC cells to the left of the slit with 7 simulated molecules and those to the right with 70 molecules. The flow develops from the intial state of rest and test conditions assigned to the low pressure region. The simulation has a Reynolds number of 10 based on the upstream speed of sound and the plate height.
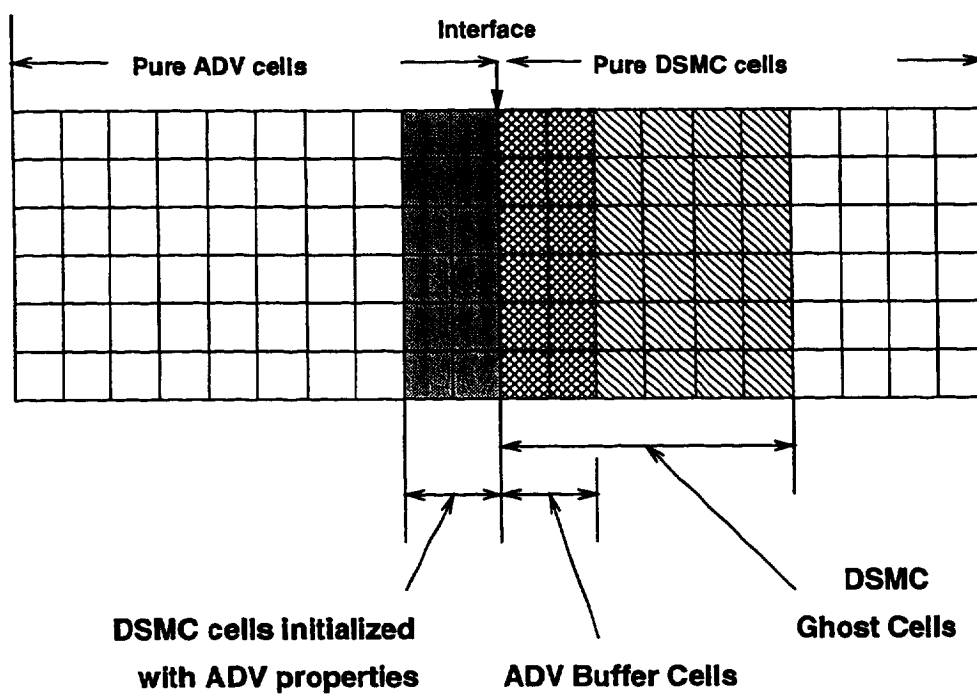
Periodic boundary conditions are applied in the vertical direction whereas absorbing boundary conditions are enforced in the horizontal direction. The solution is advanced to steady flow through 20 realizations of 100 time steps each. Fig. 5a shows pressure contours averaged over the last 4 independent realizations. The total run time was 2 hours and 15 minutes.

Choked flow exists at the throat. Pressure contours show the formation of an expansion region bounded in the vertical direction by shear layers (free boundaries) and terminated by a diffuse normal shock at x=0.24 meters. Subsequent expansion results in supersonic flow which causes the bow shock ahead of the vertical plate. Two recirculating regions arise on
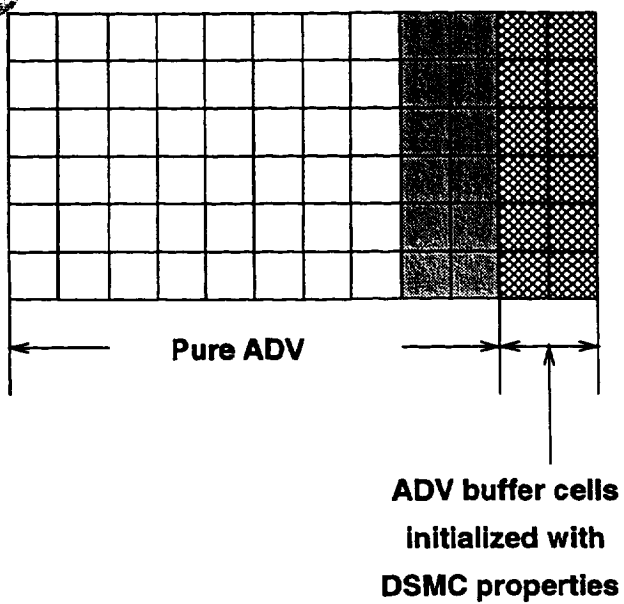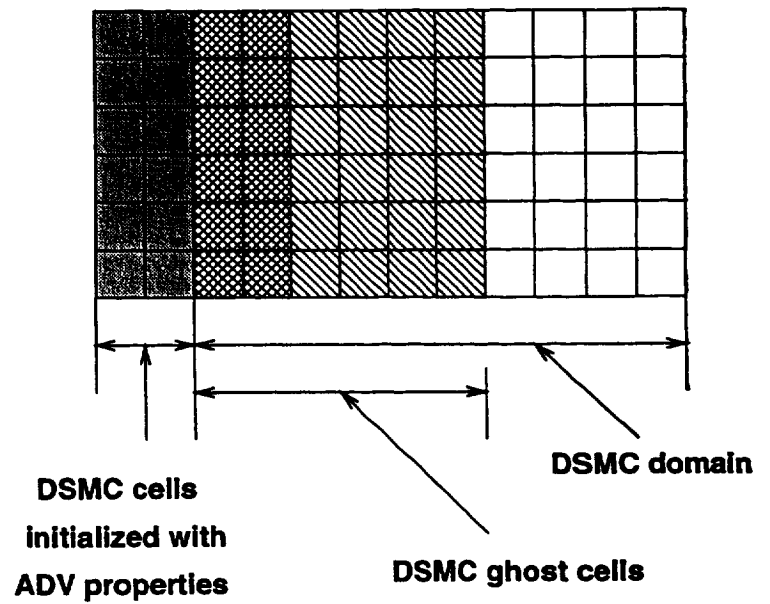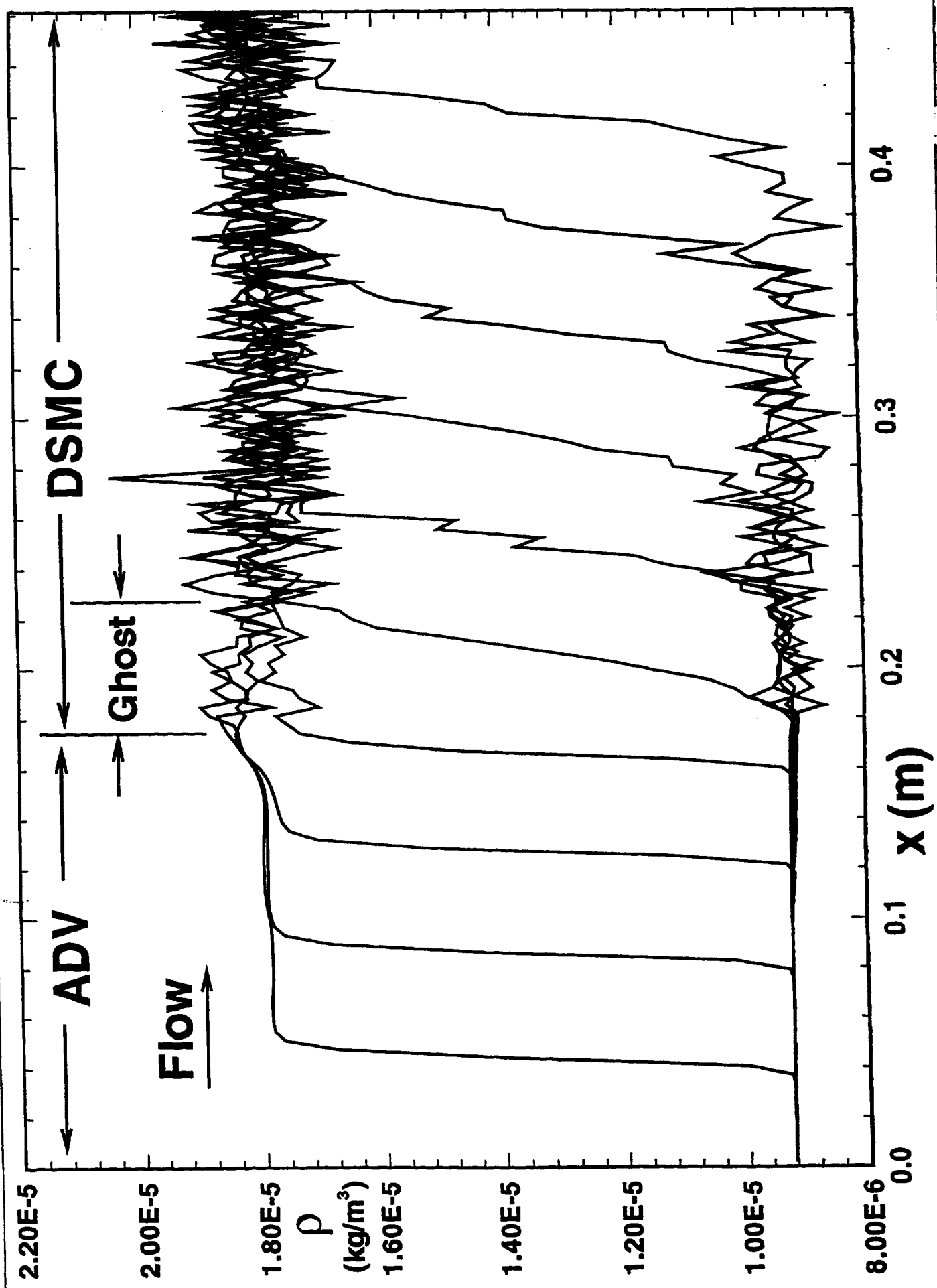
either side of the expansion region.

Interface
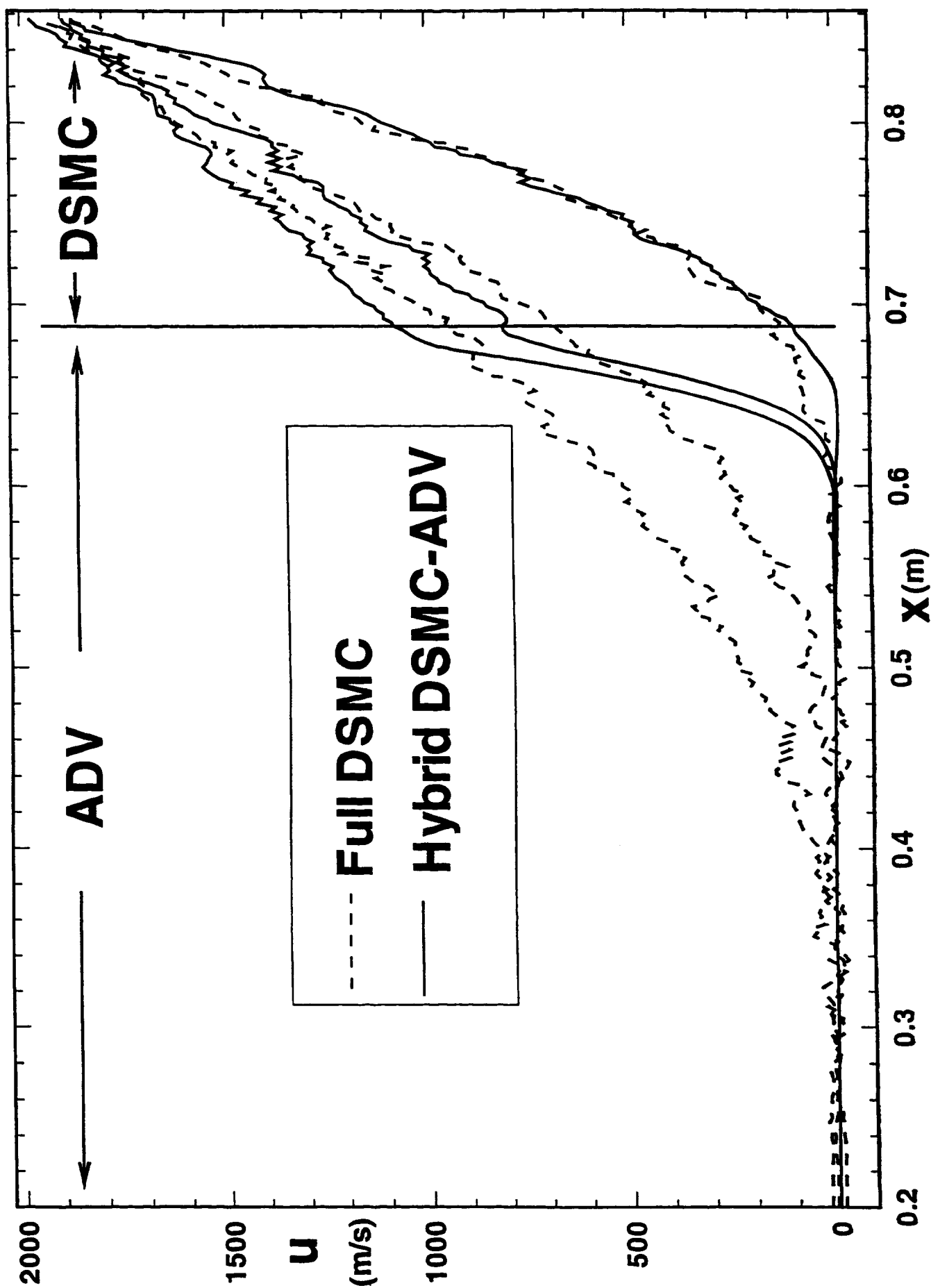
Pure ADV cells

Pure DSMC cells

DSMC cells initialized
with ADV properties

ADV Buffer Cells

**DSMC
Ghost Cells**

ADV step

DSMC step

Pure ADV

ADV buffer cells
initialized with
DSMC properties

DSMC cells
initialized with
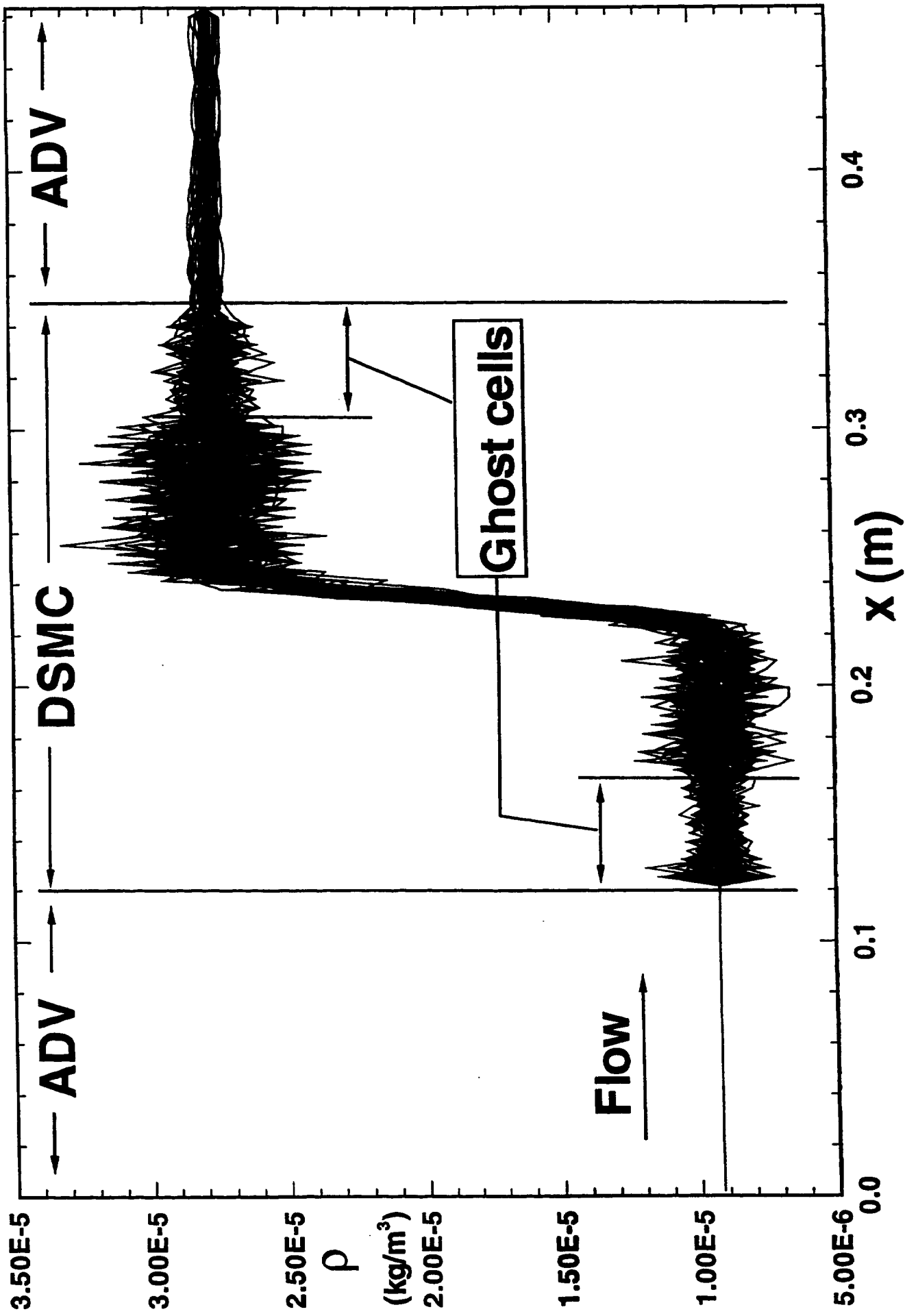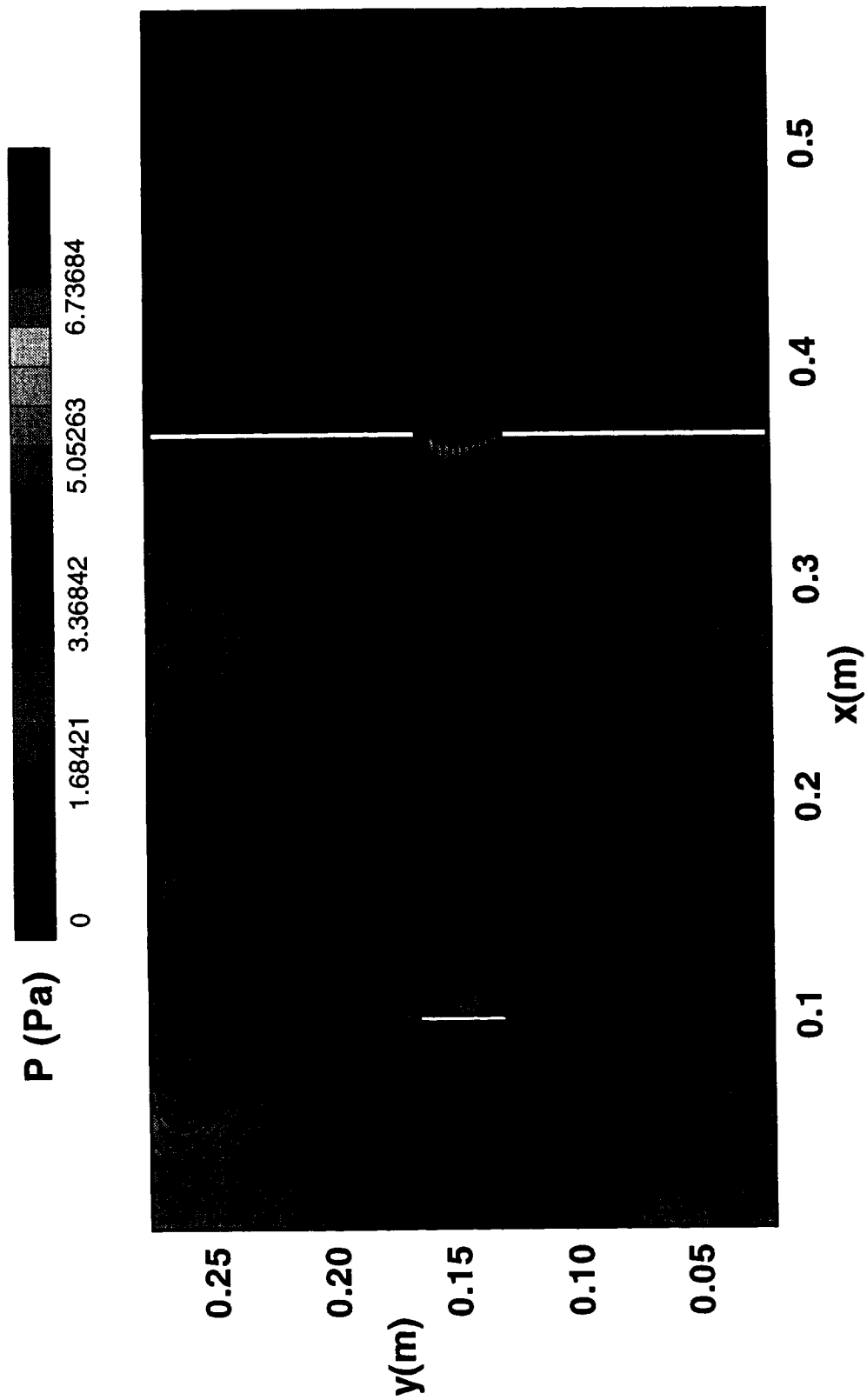ADV properties

DSMC domain

DSMC ghost cells

**Fig.1
ADV-DSMC Interface Cell Sets**

Fig. 2

Fig. 3

Fig 4

Fig. 5a

Fig. 5b